32. FILE 32, COVARIANCES OF RESONANCE PARAMETERS

32.1. General Description

File 32, MT=151, contains the variances and covariances of the resonance parameters given in File 2, MT=151. The resonance parameters, used with the appropriate resonance formulae, provide an efficient way to represent the complicated variations in the magnitudes of the different resonant partial cross sections, compared to the use of File 3 alone. Similarly for File 32, the use of the covariances of the resonance parameters of individual resonances provides an efficient way of representing the rapid variation over the individual resonances of the covariances of the partial cross sections. The covariance data of the processed cross sections include the effects of both File 32 and File 33 within a given energy region, similar to the way the cross sections themselves are the sum of contributions from File 2 and File 3.

In the resonance region, the covariances of the partial cross sections are often characterized by a) "long-range" components that affect the covariances over many resonances, and b) "short-range" components affecting the covariances of the different partial cross sections in the neighborhood of individual resonances. The former often can best be represented in File 33, while the latter can be given in File 32.

When the material composition is dilute in the nuclide of concern and the cross sections are to be averaged over an energy region that includes many resonances, the effects of "short-range" components are unimportant and the covariances of the averaged cross sections can be well represented by processing the long-range components given in File 33. Therefore, the covariances of the cross sections in the unresolved resonance energy region should be given entirely by means of File 33 unless resonance self-shielding in this energy region is thought to be of practical significance for a particular nuclide. For many nuclides these conditions may also be valid in the high-energy portion of the resolved resonance energy region.

In the resolved resonance region it may be necessary to calculate covariances for the resonance self-shielding factors to obtain the uncertainty in the Doppler effect. As another example, one may require group cross-section covariances where the groups are narrow compared to the resonance width or where only a few resonances are within a group. In these cases File 32 should be used. Because this situation may be important only in the lower energy portion of the resolved resonance region, File 32 need not include the whole set of resonances given in File 2. File 33 remains available for use in combination with File 32.

The ENDF-6 formats for File 32 are structured to maintain compatibility with those of ENDF/B-V, and there are new features to permit representation of covariance components among the parameters of different resonances. Covariances between resonance energies and widths are now also allowed. While File 32 was limited in ENDF-5 to the Breit-Wigner representations (LRF=1 or 2), in ENDF-6 formats covariances may also be given for the Reich-Moore (LRF=3) and Adler-Adler (LRF=4) formulations. A limited representation is offered for unresolved resonance parameter covariance data. The conventions are retained that the cross section covariances for the resonance region are combined from covariance data in File 32 and File 33, and that relative covariances given in File 33 apply to the cross sections reconstructed from File 2 plus File 3 when that option is specified in File 2. (There is a partial exception for LRF=4.) Since the ENDF-6 formats do not allow a continuous range of values for the total angular momentum J of a resonance, covariance data for the resonance spin are no longer recognized.

Note that File 32 formats retain many restrictions. For example, there is no provision for representing covariances between the parameters of resonances in two different materials or in two isotopes within the same elemental evaluation. Since File 32 can become cumbersome if many resonances are treated, evaluators will do so only for nuclides of greatest practical importance.

The strategy employed for File 32 is similar to that for smooth cross sections in that the variance of a resonance parameter or the covariance between two such parameters can be given as a sum of several components. Some contributions can be labeled by resonance energy and parameter type, while others can arise from long-range covariances among parameters of the same type for different resonances in the same isotope. The latter are labeled by energy bands, and the same uncertainty characteristic is applied to the indicated parameter of all the File 2 resonances in a given band.

The idea of assigning the same relative covariance to all parameters of a given type in an energy region has limited validity. One limit arises because long-range uncertainties in reaction yields don't generally carry over proportionately to uncertainties in the corresponding reaction widths. However, gamma-ray widths are sometimes known only for resonances at low neutron energy, and then the average of these values is used for the resonances at higher energy. This situation motivates formats resembling File 33 except that a relative uncertainty in the file applies to the indicated parameter (*e.g.*, Γ_γ) of every resonance in the indicated energy range. The approach here is to allow the long range correlations to extend over any energy interval in which consistent resolved resonance formulations are utilized.

The definitions of common quantities are as given in Chapter 2.

32.2. Formats

The format for File 32, MT=151, parallels the format for File 2, MT=151, with the restriction to LRF=1,2,3 or 4 for LRU=1 (resolved parameters) and to LRF=1 for LRU=2 (unresolved parameters).

The general structure of File 32 is as follows:

```
[MAT,32,151/   ZA, AWR,   0,   0, NIS,    0] HEAD
[MAT,32,151/  ZAI, ABN,   0,   0, LFW,  NER] CONT          (isotope)
[MAT,32,151/   EL,  EH, LRU, LRF, NRO, NAPS] CONT            (range)
<subsection for the first energy range for the first isotope>
[MAT,32,151/   EL,  EH, LRU, LRF, NRO, NAPS] CONT            (range)
        <subsection for the second energy range for the first isotope>
            ------------------------------
            ------------------------------
[MAT,32,151/   EL,  EH, LRU, LRF, NRO, NAPS] CONT            (range)
        <subsection for the last energy range for the first isotope>
            ------------------------------
            ------------------------------
[MAT,32,151/  ZAI, ABN,   0,   0, LFW,  NER] CONT          (isotope)
[MAT,32,151/   EL,  EH, LRU, LRF, NRO, NAPS] CONT            (range)
        <subsection for the first energy range for the last isotope>
            ------------------------------
            ------------------------------
[MAT,32,151/  EL,  EH, LRU, LRF, NRO, NAPS] CONT             (range)
        <subsection for the last energy range for the last isotope>
            ------------------------------
            ------------------------------
[MAT,32,  0/  0.0, 0.0,   0,   0,   0,    0] SEND
[MAT, 0,  0/  0.0, 0.0,   0,   0,   0,    0] FEND
```

Data are given for all ranges for a given isotope, then for successive isotopes. The data for each isotope start with a CONT (isotope) record; those for each range with a CONT (range) record. File segments need not be included for all isotopes represented in the corresponding File 2.

If the "range" record preceding a subsection has NRO≠0, indicating that the energy dependence of the scattering radius is given in File 2, the initial file segment within the subsection has the form:

```
[MAT,32,151/ 0.0, 0.0,   0,   0,   0,   NI] CONT
```
<NI sub-subsections as defined in Chapter 33.2 for the energy-dependent covariances of the scattering radius>

The next record of a subsection (the first record if NRO=0) has the form:

```
[MAT,32,151/ SPI,  AP,   0, LCOMP, NLS,  0] CONT.
```

If the compatibility flag, LCOMP, is zero, NLS is the number of L-values for which lists of resonances are given in a form compatible with that used in ENDF-5, as described in Section 32.2.1. If LCOMP=1, then NLS=0 and subsection formats are as shown in Sections 32.2.2. If LCOMP=2, the covariance matrix is expressed in compact form as described in Sect. 32.3 and 32.4.

32.2.1 Compatible resolved resonance subsection format.

This format differs from that used for ENDF-5 only in that covariances of the resonance spin are all zero. It is applicable only for resolved parameters (LRU=1) and for the Breit-Wigner formalisms (LRF=1 or 2). The following covariance quantities are defined:

DE^2	Variance of the resonance energy in units eV^2.
DN^2	Variance of the neutron width GN in units eV^2.
DNDG	Covariance of GN and GG in units eV^2.
DG^2	Variance of the gamma-ray width in units eV^2
DNDF	Covariance of GN and GF in units eV^2.
DGDF	Covariance of GG and GF in units eV^2.
DF^2	Variance of the fission width GF in units eV^2.
DJDN	(null) covariance of resonance J-value and GN.
DJDG	(null) covariance of resonance J-value and GG.
DJDF	(null) covariance of resonance J-value and GF.
DJ^2	(null) variance of resonance J-value.

A complete subsection for LCOMP = 0 has the following form:

<If NRO is not 0, a control record and NI sub-subsections for energy-dependent covariances of the scattering radius>

```
[MAT,32,151/ SPI,     AP,      0, LCOMP,     NLS,      0] CONT (LCOMP=0)
[MAT,32,151/AWRI,    0.0,      L,     0, 18*NRS,    NRS/
              ER1,    AJ1,    GT1,     GN1,     GG1,    GF1,
             DE1^2,  DN1^2, DNDG1,    DG1^2,  DNDF1,  DGDF1,
             DF1^2, DJDN1, DJDG1,  DJDF1,    DJ1^2,    0.0,
                                 (DJDN1,DJDG1,DJDF1=0.0)
```

<three physical records for each resonance through resonance NRS>] LIST

<a similar list record for each additional value of L through NLS>

Note that in this compatible format no covariance can be given between parameters of different resonances even if they overlap.

32.2.2 General resolved resonance subsection formats.

Following the record that starts with the target spin, SPI, if it states LCOMP=1, the next card of a subsection defines for that isotope and energy range how many (NSRS) sub-sections will occur for covariances among parameters of specified resonances and how many (NLRS) sub-sections are to contain data on long-range parameter covariances. The complete structure of an LCOMP=1 subsection is as follows:

```
            <f NRO≠0, a control record and NI sub-subsections for energy-
                  dependent covariances of the scattering radius>
[MAT,32,151/ SPI,  AP,   0, LCOMP,  NLS,    0] CONT   (LCOMP=1,NLS=0)
[MAT,32,151/AWRI, 0.0,   0,     0, NSRS, NLRS] CONT
            <NSRS sub-subsections each giving covariances among specified
                  parameters of enumerated sets of resonances>
            <NLRS sub-subsections each giving long-range covariances contributions
                for stated energy regions for a particular type of resonance parameter>
```

Covariance formats for NSRS-type sub-subsections

The formats here differ from the LCOMP=0 formats of Section 32.2.1 in that covariance between parameters of different resonances appear, resonance representations LRF=1 to 4 are allowed, there is no segregation by L-value, and the number of parameters considered per resonance is declared in each sub-subsection primarily to avoid tabulating zero covariances for fission widths in files concerning structural materials. The listed resonances must be present in File 2, but there is no requirement that all resonances be included in File 32 that are given in File 2.

The following paragraphs cover the formats for the NSRS sub-subsections for the various (LRF) resonance formulations for resolved parameters (LRU=1). LRF=1 through 4 are allowed.

LRF=1,2, LRU=1. These cases have the same formats. All the resonances for which covariances are to be included are divided into blocks. Covariances between parameters can only be included for resonances in the same block. (A given resonance can appear in more than one block.) A sub-subsection covers the data for a block. Within each such block, the parameters are given of those resonances for which covariances are included, and the upper triangular representation of the parameter covariance matrix is included for the whole block of resonances. For each block one specifies the number MPAR of parameters to be included for each listed resonance in the block, since for most cases there is, for example, no fission width and the size of the covariance matrix can therefore be minimized.

The NSRS-type sub-sections have the form below for LRF=1 and 2:

```
[MAT,32,151/  0.0,  0.0, MPAR,   0, NVS+6*NRB,.NRB/
```

Parameters for each resonance for which there is covariance data.

ER_1, AJ_1, GT_1, GN_1, GG_1, GF_1,
…
…
ER_{NRB}, AJ_{NRB}, GT_{NRB}, GN_{NRB}, GN_{NRB}, GG_{NRB}, GF_{NRB},

Resonance parameter

V_{11}, V_{12}, ... $V_{1,MPAR*NRB}$, V_{22},

variances and covariances for all resonances listed.	. . . ,	$V_{2,NPAR*NRB}$, V_{33},
	. . . ,	$V_{MPAR*NRB,MPAR*NB}$, 0.0, 0.0] LIST

Note that the record first lists all the parameters of resonances in the group, for positive identification, and then lists the covariance terms.

MPAR	Number of parameters per resonance in this block which have covariance data (In order: ER, GN, GG, GF, GX, indices 1-5)
NVS	Number of covariance elements listed for this block of resonances, NVS = [NRB×MPAR×(NRB×MPAR+1)]/2.
NRB	Number of resonances in this block and for which resonance parameter and covariance data are given in this sub-section.
ER	Lab system energy of the k^{th} resonance (in this block).
AJ_k	Floating-point value of the spin for the k^{th} resonance.
GT_k	Total width (eV) for the k^{th} resonance. GT=GN+GG+GF+GX.
GN_k	Neutron width of the k^{th} resonance.
GG_k	Gamma-ray width for the k^{th} resonance.
GF_k	Fission width of the k^{th} resonance.
V_{mn}	Variance (eV^2) or covariance matrix element, row m and column, n ≥ m. If j ≤ MPAR is the parameter index (j=4 for fission width) for the k^{th} resonance in the block, m = j + (k-1)×MPAR. The indexing is the order defined above under MPAR.

LRF=3, LRU=1. The representation for the Reich-Moore resonance formulation is very similar. The listing of the parameters among which covariance terms are allowed takes the form used in File 2, namely:

ER, AJ, GN, GG, GFA, GFB.

Similarly, in interpreting the indices for the covariance matrix of the parameters in a given block of resonances, the order when LRF=3 is ER, GN, GG, GFA, GFB and the largest possible value of MPAR is 5.

LRF=4, LRU=1. The Adler-Adler resonance representation includes background constants as well as resonance parameters. The uncertainty in the background constants is to be treated indirectly just as the smooth background given in File 3. (That is, in the energy region EL, EU for LRF=4 any relative uncertainty data in File 33 applies to the sum of the cross section in File 3 and the contribution of the cross sections computed from the Adler-Adler background constants. Great care will be required if this uncertainty representation for Adler-Adler fits is used in other than single-isotopes evaluations.) The inherent assumption is that covariance data will be detailed for the largest resonances, and those representing the Adler-Adler backgrounds. It is assumed that LI=7.

An LRF=4 NSRS sub-subsection takes the following form, using the previous definitions where possible:

```
[MAT,32,151/  0.0,   0.0, MPAR,    0,NVS+6*NRB,  NRB/
               DET1,  DWT1,  GRT1, GIT1,     DEF1,  DWF1,
Parameters for GRF1,  GIF1,  DEC1, DWC1,     GRC1,  GIC1,
each reference ----------------------------------
in the block.  DETNRB, DWTNRB, GRTNRB, GITNRB, DEFNRB, DWFNRB,
               GRFNRB, GIFNRB, DECNRB, DWCNRB, GRCNRB, GICNRB,
Resonance parameter V11,  V12, ----------,  V1,MPAR*NRB,    V22,
variances for all  ----------,  V2,NPAR*NRB,    V33,
resonances listed. ----------, VMPAR*NRB,MPAR*NB,      0.0,   0.0] LIST
```

The Adler-Adler parameters of the selected list of resonances are given in the same redundant style indicated in section 2.2.1.3. For LRF=4 the maximum value of MPAR is 8 and for a given resonance the covariance matrix indexing is in the order:

μ = DET = DEF = DEC, DWT = DWF = DWD = v,
GRT, GIT, GRF, GIF, GRC, GIC

Format for Long-Range Covariance Sub-subsections (LRU=1). Here are described the forms that the sub-subsections may take to represent long-range (in energy) covariances among parameters of a given type. The strategy is to use formats that resemble those for File 33 but refer to a particular parameter and equally to all resonances of a given isotope within the indicated energy regions.

Here each sub-subsection must identify the resonance parameter considered (Γ_n, Γ_γ, *etc.*) via the parameter IDP, indicate the covariance pattern via a value of LB, and give the energy regions and covariance components. The following table defines the permitted values of LB. Note the definition of one LB value not defined in File 33, and that LB=3 and 4 are not employed in File 32 because of LB=5 is typically much more convenient. The term COV[Γ_α(i),Γ_α(j)] is defined as the covariance between the Γ_α parameters for two different resonances (indexed i and j) in the same nuclide.

LB=-1 Relative variance components entirely uncorrelated from resonance-to- resonance but having constant magnitude within the stated energy intervals.

$$Cov\left[\Gamma_\alpha(i)\Gamma_\alpha(j)\right] = \delta_{ij} \sum_{k=1}^{NE-1} S_i^k \, F_{\alpha k}^{(-1)} \, \Gamma_\alpha^2(i)$$

LB=0 Absolute covariance components correlated only within each E interval.

$$Cov\left[\Gamma_\alpha(i)\Gamma_\alpha(j)\right] = \sum_{k=1}^{NE-1} P_{j,k}^{i,k} \, F_{\alpha k}^{(0)}$$

LB=1 Relative covariance components correlated only within each E interval

$$Cov\left[\Gamma_\alpha(i)\Gamma_\alpha(j)\right] = \sum_{k=1}^{NE-1} P_{j,k}^{i,k} \, F_{\alpha k}^{(1)} \, \Gamma_\alpha(i)\Gamma_\alpha(j)$$

LB=2 Fractional covariance components fully correlated over all E intervals with variable magnitude.

$$Cov\left[\Gamma_\alpha(i)\Gamma_\alpha(j)\right] = \sum_{k,k'=1}^{NE1} P_{j,k'}^{i,k} F_{\alpha k}^{(2)} F_{\alpha k'}^{(2)} \Gamma_\alpha(i)\Gamma_\alpha(j)$$

LB=5 Relative covariance components in an upper triangular representation of a symmetric matrix.

$$Cov\left[\Gamma_\alpha(i)\Gamma_\alpha(j)\right] = \sum_{k,k'=1} P_{j,k'}^{i,k} F_{\alpha kk'}^{(5)} \Gamma_\alpha(i)\Gamma_\alpha(j)$$

Note that the $F^{(-1)}$, $F^{(1)}$, and $F^{(5)}$ parameters have the dimensions of relative covariances, the $F^{(0)}$ are absolute covariances, and the $F^{(2)}$ are relative standard deviations.

The S and P are dimensionless operations defined in Section 33.2
The sub-subsection format for LB=–1, 0, 1, or 2 is:

`[MAT,32,151/  0.0,  0.0,  IDP,  LB, 2*NE,  NE/{E`$_k$`,F`$^{(LB)}$`}] LIST`

For LB=5 the requisite format is

`[MAT,32,151/  0.0,  0.0,  IDP,  LB,   NT,  NE/{E`$_k$`},{F`$_{kk}^{(5)}$`}] LIST(LB=5)`

In the above:

LB Indicator of covariance pattern as defined above.
NE Number of energies in the parameter table for a given sub-section.
NT NE*(NE+1)/2.
IDP Identification number of a resonance parameter type. This index depends on the resonance formulation used, as summarized in the table below. This table is consistent with the order of parameters used in the NSRS-type sub-subsections to define the parameter covariances included, the first NPAR parameters in the list for the given LRF value.

	LRF			
IDP	**1**	**2**	**3**	**4**
1	E_r	E_r	E_r	$E_r=\mu$
2	Γ_n	Γ_n	Γ_n	ν
3	Γ_γ	Γ_γ	Γ_γ	GRT
4	Γ_f	Γ_f	Γ_f	GIT
5	Γ_x	Γ_x	Γ_x	GRF
6				GIF
7				GRC
8				GIC

For LB=0, ±1, 2, and 5 the energy values in the tables are monotonically increasing and cover the range EL to EH. For LB=5 the F-values are given in the upper triangular representation of a symmetric matrix by rows, *i.e.* F_{11}, F_{12}, ..., $F_{1,NE-1}$; F_{22}, $F_{2,NE-1}$; $F_{NE-1,NE-1}$

32.2.3 Unresolved resonance subsection format (LRU=2)

For the unresolved resonance region a simplified covariance formulation is permitted. For the purposes of covariance representation, no energy dependence is specified for the average parameter relative covariances, even though in file 2 the unresolved region may be represented with energy-dependent average Breit-Wigner parameters using LRF=2. Relative covariance elements are tabulated, unlike the cases above.

If the evaluator wishes to represent the relative covariance of the unresolved resonance parameters, the subsection for a given isotope has the following form.

```
[MAT,32,151/  SPI,    AP,      0,     0,    NLS,     0] CONT
[MAT,32,151/ AWRI,   0.0,      L,     0, 6*NJS,   NJS/
               D1,    AJ1,   GNO1,   GG1,     GF1,   GX1,
             ----------------------------------
               DNJS, AJNJS, GNONJS, GGNJS,   GFNJS,   GXNJS] LIST
             <NJS card images for each L value in successive LIST records>
[MAT,32,151/  0.0,   0.0, MPAR,    0,(NPAR*(NPAR+1))/2,NPAR/
               RV11, RV12, -------------------------,
             -----------, RV1,NPAR,--------, RNNAPR,NPAR] LIST
```

MPAR is the number of average parameters for which relative covariance data are given for each L and J, in the order D, GNO, GG, GF, and GX, for a maximum of 5. That is, relative covariance values for the first MPAR of these are tabulated for each (L,J) combination. If MPAR is given as 4 when LFW=0 on the CONT (isotope) record, then the four covariance matrix indices per (L,J) combination represent D,GNO, GG, and GX.

NPAR=MPAR∗(sum of the values of NJS for each L).

The LSSF flag is defined in Section 2.3.1.

RV_{ij}, the relative covariance quantities among these average unresolved parameters for the given isotope. The final LIST record contains the upper triangular portion of the symmetric relative covariance matrix by rows.

32.3. General Description of Compact Covariance Matrix.

This format was developed in order to provide a means of communicating the actual resonance-parameter covariance matrix (as determined during the data-evaluation process) in a compact, legible, and accurate form, for those situations in which it is not practical to provide the entire covariance matrix using the LCOMP=1 format. The covariance matrix is specified as uncertainties plus correlation matrix. The correlation coefficients (whose values range from -1 to 1) are presented in a compact representation; each approximated correlation coefficient differs from the original value by at most 0.005.

If the covariance matrix element connecting parameter number *i* with parameter number *j* is denoted by V_{ij}, the uncertainty on parameter *i* by D_i, and the correlation coefficient by C_{ij}, then these quantities are related by

$D_i^2 = V_{ii}$ $\qquad\qquad$ $V_{ij} = D_i C_{ij} D_j$

Values for C_{ij} range from -1 to +1; values for D_i are always positive. Note that the diagonal elements of C_{ij}, those for which $i = j$, are always exactly 1.0 and therefore are never specified explicitly. Compacting the off-diagonal correlation coefficients is accomplished as follows:

1. Drop (set to zero) all values of C_{ij} between -0.02 and +0.02.
2. Multiply the remaining coefficients by 100.
3. Map all positive values greater than K and less than or equal to K+1 to the integer K.
4. Map all negative values less than -K and greater than or equal to -K-1 to the integer -K.

The reverse mapping takes the integer to the center of the range. For example, the positive integer 87 (which corresponds to original correlation coefficients in the range from 0.87 up to and including 0.88) maps to 0.875. The negative integer -12 (which corresponds to original correlation coefficients in the range from -0.12 inclusive down to -0.13 exclusive) maps to correlation coefficient -0.125.

Two types of records are used to read the mapped correlation coefficients. A CONT record defines NNN (the number of parameters) and NM (the number of lines of INTG records that follow).

```
[MAT,  32,  151 /  0.0,  0.0,  0,  NNN,  NM,  NM]   CONT
[MAT,  MF,  MT / II,  JJ,  KIJ  ]  INTG
[MAT,  MF,  MT / II,  JJ,  KIJ  ]  INTG
```

< Continue until a total of NM INTG records are read >

The information stored in the INTG records may be summarized as follows: Let i and j represent two of the parameters in the numbering scheme defined above, with $i > j$. All those correlation coefficients mapped to non-zero integers K_{ij} are printed in File 32; zero-valued K_{ij} are printed (as blanks or zeros) only when they occur on the same record with non-zero values. Each line (record) in the file begins by specifying the location (i.e., by specifying i and j, with $i > j$); other K=s on the same line correspond to $(i, j+1)$, $(i, j+2)$, ... $(i, j+17)$ [so long as $j + 17 < i$]. If there are more non-zero K=s for the same i, they are given on another line, again beginning with the next non-zero K.

The following FORTRAN can be used to read the mapped correlation coefficients and reconstruct the correlation matrix:

```
      DIMENSION K(18), CORR(n,n)
C     Note that n must be greater than or equal to NNN
      READ (LIB,10) NNN, NM, NX, MAT, MF, MT, NS
   10 FORMAT (33X, 3I11, I4, I2, I3, I5)
C     The CONT record: NNN is dimension of CORR(NNN,NNN), and
C             NM is the number of lines to follow in the file
      DO I=1,NNN
         DO J=1,I-1
            CORR(J,I) = 0.0
```

```
        END DO
        CORR(I,I) = 1.0
      END DO
      DO M=1,NM
        READ (LIB,20) I, J, (K(N),N=1,18), MAT, MF, MT, NS
   20   FORMAT (I5, I5, 1X, 18I3, 1X, I4, I2, I3, I5)
C       This is the INTG record
        JP = J - 1
        DO N=1,18
          JP = JP + 1
          IF (JP.GE.I) GO TO 30
          IF (K(N).NE.0) THEN
            IF (K(N).GT.0) THEN
              CORR(JP,I) = (K(N)+0.5)/100.0
          ELSE
            CORR(JP,I) = - (-K(N)+0.5)/100.0
          END IF
        END IF
      END DO
   30 CONTINUE
       END DO
```

Note that only the upper-triangular portion of the correlation matrix [CORR(J,I) for J < I] is defined by this procedure. The lower-triangular portion can be found by invoking symmetry [CORR(I,J) = CORR(J,I)].

32.4 Formats for Compact Covariance Matrix

The compact format for covariances uses File 32, MT=151, with LCOMP = 2 (with LRF = 1, 2, 3, and 7) for LRU=1 (resolved-resonance parameters). The format parallels the format for File 2, MT = 151, with parameter uncertainties specified along with parameter values. Correlation coefficients are given separately.

The general structure of File 32 is as given in Section 32.2.

```
[MAT, 32, 151 /  ZA, AWR,   0,   0, NIS,    0]HEAD
[MAT, 32, 151 / ZAI, AWR,   0, LFW, NER,    0]CONT (isotope)
[MAT, 32, 151 /  EL,  EH, LRU, LRF, NIS, NAPS]CONT  (range)
  <subsection for the first energy range for the first isotope>
[MAT, 32, 151 /  EL,  EH, LRU, LRF, NIS, NAPS]CONT  (range)
  <subsection for the second energy range for the first isotope>
  ---------------------------------------------------------------------
  ---------------------------------------------------------------------
[MAT, 32, 151 /  EL,  EH, LRU, LRF, NIS, NAPS]CONT  (range)
  <subsection for the last energy range for the first isotope>
  ---------------------------------------------------------------------
  ---------------------------------------------------------------------
[MAT, 32, 151 / ZAI, AWR,   0, LFW, NER,    0]CONT (isotope)
[MAT, 32, 151 /  EL,  EH, LRU, LRF, NIS, NAPS]CONT  (range)
  <subsection for the first energy range for the last isotope>
  ---------------------------------------------------------------
  ---------------------------------------------------------------
[MAT, 32, 151 /  EL,  EH, LRU, LRF, NIS, NAPS]CONT  (range)
  <subsection for the last energy range for the last isotope>
[MAT, 32,   0 / 0.0, 0.0,   0,   0,   0,    0]SEND
[MAT,  0,   0 / 0.0, 0.0,   0,   0,   0,    0]FEND
```

Formats for the individual subsections differ depending on the value of LRF, and are discussed in Sections 32.4.1.

32.4.1 Compact covariance matrix formats for subsections of a particular energy range and isotope

In the format descriptions to follow, the notation is as defined in Section 2. Uncertainties are denoted by parameters whose names begin with AD@ but are otherwise identical to the parameter of Section 2. For example, ER represents the resonance energy in the laboratory system, in units of eV. Therefore, DER represents the uncertainty (square root of the variance) associated with the resonance energy; DER has the same units as ER.

Parameters which are not variables (that is, which are not searchable parameters in the analysis process) do not have uncertainties associated with them. For example, the total spin of a resonance, denoted by parameter AJ, has no associated uncertainty DAJ. In File 32, the value 0.0 is given instead of DAJ (for LRF = 1,2,3).

For LRF = 1 and 2, the redundant parameter GT (which is equal to GN + GG + GF) has no corresponding uncertainty DGT specified explicitly. Instead, if needed, DGT may be calculated using values for DGN, DGG, and DGF, and the correlation matrix.

During the evaluation process, not all potential variables are treated as searchable parameters. For example, if no capture cross section data were available, the evaluator might choose to set all capture widths GG to a constant value. The associated uncertainty DGG is then specified in File 32 as -1.0, indicating that this parameter=s uncertainty is not known. (The proper procedure to be used in evaluating the effect of these unvaried parameters on the final covariance matrix remains an open question, and is not addressed in this document.)

In order to express the correlation matrix as compactly as possible, the resonance parameters (those which may be varied during the evaluation process) are implicitly numbered, in the order in which they occur in the listing of File 2. For LRF = 1, 2, or 3, the non-searchable parameter AJ is included in the list but is NOT included in this numbering, nor (for LRF=1 or 2) is the redundant parameter GT. Parameters whose value is given but whose uncertainty is unknown (as described in the previous paragraph) are nevertheless included in the numerical ordering. For completely non-fissile nuclides, fission widths are not included in the numbering scheme; likewise, for fissile or fissionable nuclides for which the evaluator chose to use only one fission width, the second fission width (for LRF = 3) would not be counted.

Notation used here not previously defined:

NRSA Total number of resonances for all L values

32.4.1.2 SLBW and MLBW (LRU=1, LRF=1 or 2)

The structure of the *subsection* (assuming NRO = 0) is:

```
[MAT, 32, 151 / SPI,  AP,     0,LCOMP,   NLSA,    0]CONT
[MAT, 32, 151 /AWRI,  QX,     0,    0,12*NRSA, NRS /
             ER1,  AJ1,   GT1,   GN1,    GG1,  GF1,
            DER1, 0.0 ,   0.0,  DGN1,   DGG1, DGF1,
             ER2,  AJ2,   GT2,   GN2,    GG2,  GF2,
            DER2, 0.0 ,   0.0,  DGN2,   DGG2, DGF2,
            ----------------------------------------
             ERNRS, AJNRS, GTNRS,   GNNRS,  GGNRS, GFNRS
            DERNRS, 0.0,    0.0, DGNNRS, DGGNRS, DGFNRS  ] LIST
[MAT, 32, 151 / 0.0,  0.0,     0,   NNN,    NM, 0    ] CONT
[MAT,  MF,  MT / II, JJ, KIJ ] INTG
[MAT,  MF,  MT / II, JJ, KIJ ] INTG
```

< Continue until a total of NM INTG records are read >

Note that NNN is the total number of unique resonance parameters included in this listing, not including AJ or GT. For fissile nuclides, NNN = NRS H 4; for non-fissile nuclides, NNN = NRS H3.

32.4.1.3 Reich Moore Limited (LRU=1, LRF=7)

The structure of the *subsection* is

```
[MAT, 32, 151/ SPI,  AP,     LAD,  LCOMP, NLS,  NLSC]CONT
[MAT, 32, 151/AWRI,    0,    0,    0,     12*NRSA,NRSA /
           ER1,   AJ1,  GN1,  GG1,  GFA1,  GFB1,
           DER1,  0.0 , DGN1, DGG1, DGFA1, DGFB1,
           ER2,   AJ2,  GN2,  GG2,  GFA2,  GFB2,
           DER2,  0.0 , DGN2, DGG2, DGFA2, DGFB2,
           ------------------------------------------------
           ERNRS, AJNRS, GNNRS, GGNRS, GFANRS, GFBNRS,
           DERNRS,0.0,  DGNNRS,DGGNRS, DGFANRS, DGFBNRS     ]LIST
[MAT, 32, 151 /   0.0,  0.0,  0,    NNN,   NM,   0   ]CONT
[MAT,  MF,  MT / II, JJ, KIJ ] INTG
[MAT,  MF,  MT / II, JJ, KIJ ] INTG
```

< Continue until a total of NM INTG records are read >

Note that NNN is the total number of resonance parameters in this listing (again not including AJ). For non-fissile nuclides, NNN = NRSA H 3. For fissile nuclides, NNN = NRSA H 4 if only one fission channel is used, and NNN = NRSA H 5 if both are used.

32.4.1.3 Reich Moore Limited (LRU=1, LRF=7)

The structure of the *subsection* is

```
[MAT,32,151/ 0.0,  0.0,     0,LCOMP,    NJS,    0     ] CONT
[MAT,32,151/ 0.0,  0.0,   NPP,    0, 12*NPP,   2*NPP/
            MA1,   MB1,    ZA1,   ZB1,    IA1,     IB1,
             Q1,  PNT1,   SHF1,   MT1,    PA1,     PB1,
            MA2,   MB2,    ZA2,   ZB2,    IA2,     IB1,
             Q2,  PNT2,   SHF2,   MT2,    PA2,     PB1,
           ------------------------------------------------
            ANPP,  MBNPP,   ZANPP,  ZBNPP,   IANPP,   IBNPP,
            QNPP, PNTNPP,  SHFNPP,  MTNPP,   PANPP,   PBNPP   ] LIST
[MAT,32,151/  AJ,  PJ,      0,     0,  6*NCH,   NCH/
           IPP1,   L1,     SCH1,  BND1,   APE1,   APT1,
           IPP2,   L2,     SCH2,  BND2,   APE2,   APT2,
           ------------------------------------------------
           IPPNCH, LNCH,   SCHNCH, BNDNCH,  APENCH,  APTNCH   ] LIST
           ------------------------------------------------
[MAT,32,151/0.0,    0.0,      0,      NRS,  12*NX,  NX/
           R1,  GAM1,1,  GAM2,1,  GAM3,1,  GAM4,1, GAM5,1,
           GAM6,1,      ...,   GAMNCH,1,
           DER1, DGAM1,1, DGAM2,1, DGAM3,1, DGAM4,1,DGAM5,1,
           DGAM6,1,      ...,  DGAMNCH,1,
           ER2,  GAM1,2, GAM2,2,   GAM3,2,  GAM4,2, GAM5,2,
           GAM6,2,      ...,   GAMNCH,2,
           DER2, DGAM1,2, DGAM2,2, DGAM3,2, DGAM4,2,DGAM5,2,
           DGAM6,2,      ...,  DGAMNCH,2,
           ------------------------------------------------
           ERNRS, GAM1,NRS, GAM2,NRS, GAM3,NRS, GAM4,NRS, GAM5,NRS,
           GAM6,NRS,     ...,   GAMNCH,NRS
           DERNRS,DGAM1,NRS,DGAM2,NRS,DGAM3,NRS,DGAM4,NRS,DGAM5,NRS,
           DGAM6,NRS,     ...,  DGAMNCH,NRS                    ] LIST
```

<The above two list records are repeated until each of the NJS J^{π} states has been specified.>

```
[MAT,  MF,  MT / II, JJ, KIJ ] INTG
[MAT,  MF,  MT / II, JJ, KIJ ] INTG
```

< Continue until a total of NM INTG records are read >

For LRF = 7 (unlike other formats), the number of channels may vary from one spin group to another. The number of resonance parameters NNN is therefore given by the sum (from 1 to NJS) of (NCH H NRS).

32.5 Procedures

As indicated earlier, it is desirable to utilize File 32 when self shielding is important or when only a few resonances fall within an energy group of the processed cross sections. It is believed that in most cases the covariances the evaluator needs to represent will not use many of the available File 32 options. One does not expect to find covariance data in File 32 for all the resonance parameters in File 2.

Correspondence Between Files 2 and 32. Completeness of File 32.

1. The overall energy range for a given isotope in File 32 is nested within the corresponding range of File 2. In either case, there may be several energy range control records. The following rules apply separately for each isotope:

   a. The smallest lower range limit EL for files 2 and 32 must agree.

   b. The highest upper range limit EH for File 32 may be smaller than or equal to that for File 2.

   c. In file 32 as in File 2, the energy ranges of the subsections may not leave gaps. Subsections with LRU=1 may overlap if consistent resonance formulations are referenced (LRF=1 or 2).

   d. An unresolved energy region (LRU=2) may be used in File 32 if one is employed in File 2. If one is used, its lower energy range limit must equal the corresponding limit for File 2.

2. In a file 32 LCOMP=0 subsection, any selection of the resonances shown in File 2 with LRF=1 or 2 must be listed in order of increasing energy. The resonance energy given in File 32 shall agree with that in File 2 for the same resonance to a relative tolerance of $\leq 10^{-5}$ to assume positive identification.

3. In LCOMP=1, LRU=1 subsections, any selection of the resonances shown in File 2 for consistent resonance formulations may be listed in NSRS-type sub-subsections. The listed resonances should be in order of increasing energy within each block, and the blocks should be arranged by order of increasing energy for the lowest-energy resonance in the block. A given resonance may appear in more than one block. The resonance energy given in File 32 shall agree with that in File 2 for the same resonance to a relative tolerance of $\leq 10^{-5}$.

4. The energy identifiers of every NLRS-type sub-subsection must cover the entire energy range (EL,EH) of the subsection. However, any desired covariance components may be null.

5. NLRS-type sub-subsections may be included in any order in LCOMP=1, LRU=1 subsections.

Obtaining Cross Section Covariances From File 32 and File 33.

1. Outside the combined energy range covered by File 32, whether in part or all of the energy range covered by File 2, the covariance data in File 33 refers to the cross sections reconstituted from File 2 plus File 3 according to the value of the LSSF flag.

2. In LCOMP=0 subsections a non-zero variance or covariance involving the resonance spin J (AJ) will be treated as null.

3. When File 32 is present for a resolved resonance range (LRU=1), the covariances among the effective cross sections in the region are obtained by combining data from Files 32 and 33.

   a. A resonance parameter covariance matrix is developed by summing all the contributions for

each resonance from the File 32 subsections with LRU=1.

b. The resonance parameter covariance file is processed to obtain the covariance data of effective cross sections implied by File 32. (This data will in general be a function of isotopic dilution and temperature.) Covariance for the various isotopes are summed with appropriate weights if the evaluation is an "elemental" one.

c. Covariances derived from File 32 are summed with those given in File 33. With one exception, relative covariances given in File 33 apply to the effective cross sections reconstituted from File 2 and File 3. In that exception, when the Adler-Adler (LRF=4) resonance formulation is employed, any relative covariances in File 33 for that energy region apply to the sum of the cross section from File 3 with the smooth background given for the LRF=4 resonance data.

4. When File 32 is present for the unresolved resonance range (LRU=2), covariance data for the region are obtained as follows:

   a. File 33 covariance data for this energy region are taken to represent the covariances of evaluated average cross sections for "infinite isotopic dilution."

   b. To obtain covariances among effective cross sections for material dilutions such that uncertainties in self shielding can become important, the effects of the unresolved resonance parameter covariances in File 32 and the evaluated average cross section covariances in File 33 are to be combined. A means for this combination was described by deSaussure and Marable [Ref. 1]. (Note that covariances of the effective cross sections in one test case were not much affected by uncertainties in average parameters. See B.L. Broadhead and H.L. Dodds [Ref. 2].)

Example For Mat 3333.

The nucleus of concern in this example has resonances represented by LRF=2 for the energy range (1,50). Five (5) resonances are given in File 2, one of which lies at negative energy, but the resonance at 15 eV is considered only relative to long-range uncertainties. Table 32.1 shows the File 2 for the example, and Table 32.2 shows the corresponding file 32.

In File 32, there are included three NSRS-type sub-subsections and four NLRS-type sub-subsections. Of the former, the first refers only to the negative energy resonance and indicates the following parameter covariance contribution for that resonance, in eV^2

E_r	1.0	-1.5	0	-0.2
Γ_n	-1.5	4.0	0	-1.0
Γ_γ	0	0	0	0
Γ_f	-0.2	-1.0	0	0.8

This block is mostly to express the negative correlation between neutron width and apparent resonance energy for this guessed resonance.

The second sub-subsection refers only to the 5-eV resonance, and conveys the following covariance contribution:

E_r	0.5×10^{-6}	0	0	0
Γ_n		1×10^{6}	1×10^{6}	0.2×10^{6}
Γ_γ		1×10^{6}	0.0	2.0×10^{6}
Γ_f		0.2×10^{6}	2.0×10^{6}	4×10^{6}

The third block covers Γ_n covariances for the 30 and 40 eV resonances.

The first NLRS sub-subsection gives the Γ_γ uncertainty correlated among all the resonances. The value is assumed to have been determined solely by analysis of the 5-eV resonance. Note that the variance for the 5-eV resonance generated by the sub-subsection fills the "hole" in the table just above (with the value 16×10^{-6}). The second sub-subsection expresses the expected resonance-to-resonance uncorrelated fluctuation in Γ_γ. The third and fourth sub-subsections cover long-range uncertainties in Γ_n and Γ_f - the example for the former might be hard for the evaluator to defend for a real nuclide.

Example 32.1. File 2 for Sample of File 32

```
99.280+3   2.70 +2         0         0    NIS=1         0333332151 HEAD
99.280+3   1.00 +0         0     LFW=0    NER=1         0333332151 CONT
   1. +0   5.00 +1     LRU=1     LRF=2    NRO=0    NAPS=0333332151 CONT
  1.0 +0   0.6  +0         0         0    NLS=1         0333332151 CONT
  2.7 +2   0.0  +0       L=0     LRX=0 6*NRS=30     NRS=5333332151
 .1.0 +0   1.5  +0  4.04 +0   3.0  +0   0.04 +0   1.0  +0333332151
  5.0 +0   1.5  +0  0.07 +0   0.01 +0   0.04 +0   0.02 +0333332151
  1.5 +1   0.5  +0  0.08 +0   0.01 +0   0.04 +0   0.03 +0333332151
  3.0 +1   1.5  +0  7.04 +0   1.0  +0   0.04 +0   6.0  +0333332151
  4.0 +1   1.5  +0  6.04 +0   5.0  +0   0.04 +0   1.0  +0333332151 LIST
  0.0 +0   0.0  +0         0         0         0         0333332  0 SEND
  0.0 +0   0.0  +0         0         0         0         03333 0  0 FEND
```

Example 32.2. Sample File 32

```
99.280+ 3  2.70 + 2         0         0    NIS=1         0333332151 HEAD
99.280+ 3  1.00 + 0         0    LFW=0    NER=1         0333332151 CONT
   1. + 0  5.00 + 1    LRU=1    LRF=2    NRO=0   NAPS=0333332151 CONT
  1.0 + 0  0.6 + 0          0  LCOMP=1    NLS=0         0333332151 CONT
  2.7 + 2  0.0 + 0          0         0   NSRS=3   NLRS=4333332151 CONT
  0.0 + 0  0.0 + 0    MPAR=4                 16*   NRB=1333332151
 -1.0 + 0  1.5 + 0  4.04 + 0  3.0 + 0 0.04 + 0  1.0 + 0333332151
  1.0 + 0 -1.5 + 0   0.0 + 0 -0.2 + 0  4.0 + 0  0.0 + 0333332151
 -1.0 + 0  0.0 + 0   0.0 + 0  0.8 + 0  0.0 + 0  0.0 + 0333332151 LIST
  0.0 + 0  0.0 + 0    MPAR=4                 16*   NRB=1333332151
  5.0 + 0  1.5 + 0  0.07 + 0 0.01 + 0 0.04 + 0 0.02 + 0333332151
  0.5 - 6  0.0 + 0   0.0 + 0  0.0 + 0  1.0 - 6  -1.0 -6333332151
 -0.2 - 6  0.0 + 0  -2.0 - 6  4.0 - 6  0.0 + 0  0.0 + 0333332151 LIST
  0.0 + 0  0.0 + 0    MPAR=2                 22*   NRB=2333332151
  3.0 + 1  1.5 + 0  7.04 + 0  1.0 + 0  0.04 + 0 6.0 + 0333332151
  4.0 + 1  1.5 + 0  6.04 + 0  5.0 + 0  0.04 + 0 1.0 + 0333332151
  2.0 - 3  0.0 + 0   0.0 + 0  0.0 + 0  1.0 - 3  0.0 + 0333332151
 -0.5 - 4  2.0 - 3   0.0 + 0  2.0 - 3  0.0 + 0  0.0 + 0333332151 LIST
  0.0 + 0  0.0 + 0     IDP=3     LB=1   2*NE=4     NE=2333332151
 -2.0 + 0  1.0 - 2   5.0 + 1  0.0 + 0  0.0 + 0  0.0 + 0333332151 LIST
  0.0 + 0  0.0 + 0     IDP=3    LB=-1   2*NE=8     NE=4333332151
 -2.0 + 0  1.0 - 2   1.0 + 0  0.0 + 0  1.0 + 1  1.0 - 2333332151 LIST
  5.0 + 1  0.0 + 0   0.0 + 0  0.0 + 0  0.0 + 0  0.0 + 0333332151 LIST
  0.0 + 0  0.0 + 0     IDP=2     LB=5     NT=6     NE=3333332151
  1.0 - 5  2.0 + 1   5.0 + 1  1.0 - 4  1.0 - 4  2.0 - 4333332151 LIST
  0.0 + 0  0.0 + 0     IDP=4     LB=1   2*NE=4     NE=2333332151
  1.0 - 5  4.0 - 4   5.0 + 1  0.0 + 0  0.0 + 0  0.0 + 0333332151 LIST
  0.0 + 0  0.0 + 0          0         0         0         0333332  0 SEND
  0.0 + 0  0.0 + 0          0         0         0         03333 0  0 FEND
```

REFERENCES

1. G. DeSaussure and Marable, ***Nucl. Sci. Eng.*** **101**, 285 (1989)
2. B. L. Broadhead and H. L. Dodds, ***Trans. Am. Nucl. Soc.*** **39**, 929 (1981)

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